Berry's phase

Let us investigate how the final state differs from the initial state if the parameters in the Hamiltonian are carried adiabatically around some closed cycle.

In the previous lecture we found out that a particle which starts in the n-th state of $H(t=0)$ remains in the n-th state of $H(t)$, picking up only a phase factor:

$$\Psi_n = e^{i[\theta_n(t)+\gamma_n(t)]}\,\psi_n(t)$$

where

$$\theta_n(t) = -\frac{1}{\hbar}\int_0^t E_n(t')\,dt' \quad \text{— dynamic phase}$$

and

$$\gamma_n(t) = i\int_0^t \left\langle \psi_n(t') \middle| \frac{\partial}{\partial t'}\psi_n(t') \right\rangle dt' \quad \text{— geometric phase}$$

Now suppose $\psi_n(t)$ depends on t through some parameter $R(t)$. Thus,

$$\frac{\partial \psi_n}{\partial t} = \frac{\partial \psi_n}{\partial R}\frac{dR}{dt}$$

and

$$\gamma_n(t) = i\int_0^t \left\langle \psi_n \middle| \frac{\partial \psi_n}{\partial R} \right\rangle \frac{dR}{dt'}\,dt' = i\int_{R_i}^{R_f} \left\langle \psi_n \middle| \frac{\partial \psi_n}{\partial R} \right\rangle dR$$

where R_i and R_f are the initial and final values of $R(t)$. If $R_f(T) = R_i(0)$ then $\gamma_n(T) = 0$

However, if we assume that there is more than one parameter (say N of them) then

$$\frac{\partial \varphi_n}{\partial t} = \frac{\partial \varphi_n}{\partial R_1}\frac{dR_1}{dt} + \frac{\partial \varphi_n}{\partial R_2}\frac{dR_2}{dt} + \dots + \frac{\partial \varphi_n}{\partial R_N}\frac{dR_N}{dt} = (\nabla_{\vec{R}}\varphi_n)\cdot\frac{d\vec{R}}{dt}$$

$$\vec{R} = \begin{pmatrix} R_1 \\ R_2 \\ \vdots \\ R_N \end{pmatrix} \qquad \nabla_R = \begin{pmatrix} \frac{\partial}{\partial R_1} \\ \frac{\partial}{\partial R_2} \\ \vdots \\ \frac{\partial}{\partial R_N} \end{pmatrix}$$

and

$$\gamma_n(t) = i\int_{\vec{R}_i}^{\vec{R}_f} \langle \varphi_n | \nabla_{\vec{R}} \varphi_n \rangle \cdot d\vec{R}$$ (here $d\vec{R}$ stands for a vector)

If the Hamiltonian returns to its original form after a time T, the net geometric phase change is:

$$\gamma_n(T) = i\oint \langle \varphi_n | \nabla_{\vec{R}} \varphi_n \rangle \cdot d\vec{R}$$

It should be noted that $\gamma_n(T)$ depends on the path only (in the space of parameters R_i), not on how fast the path is traversed. In contrast

$$\theta_n(T) = -\frac{1}{\hbar}\int_0^T E_n(t')\,dt'$$

Despite γ_n being just a phase factor it may be measurable. Suppose a beam of particles (all in state Ψ) is split in two and then one of them is passed through an adiabatically changed potential. Then when the two beams are recombined, the total wave function has the form

$$\Psi = \frac{1}{2}\Psi_0 + \frac{1}{2}\Psi_0 e^{i\Gamma}$$ when Γ is the extra phase (in part dynamic and in part geometric)

$$|\Psi|^2 = \frac{1}{4}|\Psi_0|^2 (1+e^{i\Gamma})(1+e^{-i\Gamma}) = \frac{1}{2}|\Psi_0|^2(1+\cos\Gamma) =$$

$$= |\Psi_0|^2 \cos^2\frac{\Gamma}{2}$$

When the parameter space is 3-dimensional, $\vec{R} = (R_1, R_2, R_3)$, Berry's formula looks similar to the expression for magnetic flux

$$\Phi = \int_S \vec{B} \cdot d\vec{s}$$

If we write the magnetic field as $\vec{B} = (\nabla \times \vec{A})$ and use the Stoke's theorem

$$\Phi = \int_S (\nabla \times \vec{A}) \cdot d\vec{s} = \oint_C \vec{A} \cdot d\vec{\ell}$$

Thus Berry's phase can be thought of as the "flux" of a "magnetic field"

$$\vec{B} = i \nabla_{\vec{R}} \times \langle \varphi_n | \nabla_{\vec{R}} \varphi_n \rangle$$

through the closed loop trajectrory in parameter space.

$$\gamma_n(T) = i \int_S \left[\nabla_{\vec{R}} \times \langle \varphi_n | \nabla_{\vec{R}} \varphi_n \rangle \right] \cdot d\vec{s}$$

Let us work through an example of the concept of the Berry phase. Imagine an electron at origin subjected to a magnetic field that is constant in magnitude but whose direction precesses around the z-axis (making a fixed angle α) with angular velocity ω. The exact solution (which we also used in the last lecture) is given by

$$\chi(t) = \left[\cos\frac{\lambda t}{2} - i\,\frac{(\omega_0 - \omega\cos\alpha)}{\lambda}\sin\frac{\lambda t}{2}\right] e^{-\frac{i\omega t}{2}}\,\chi_+(t)$$
$$+\, i\left[\frac{\omega}{\lambda}\sin\alpha\,\sin\frac{\lambda t}{2}\right] e^{\frac{i\omega t}{2}}\,\chi_-(t)$$

$$\lambda = \sqrt{\omega^2 + \omega_0^2 - 2\omega\omega_0\cos\alpha} \qquad \omega_0 = \frac{eB_0}{m} \qquad E_\pm = \pm\frac{\hbar\omega_0}{2}$$

If $\omega \ll \omega_0$ then $\lambda \simeq \omega_0 - \omega\cos\alpha$

and

$$\chi(t) \approx e^{-\frac{i\omega_0 t}{2}}\, e^{i\frac{\omega\cos\alpha\, t}{2}}\, e^{-\frac{i\omega t}{2}}\,\chi_+(t) + i\,\frac{\omega}{\omega_0 - \omega\cos\alpha}\sin\alpha\,\sin\frac{\omega_0\lambda}{2}\Big]\, e^{\frac{i\omega t}{2}}\,\chi_-(t)$$

When $\frac{\omega}{\omega_0} \to 0$ the coefficient by $\chi_-(t)$ vanishes and we get what we are supposed to according to the adiabatic theorem : $\Psi_n(t) = e^{i\theta_n(t)}\, e^{i\gamma_n(t)}\,\psi_n(t)$ - the system stays in the state where it began, $\chi_+(t)$. At the same time

$$\theta_+(t) = -\frac{1}{\hbar}\int_0^t E_+(t')\,dt' = -\frac{\omega_0 t}{2}$$

Then the geometric phase is

$$\gamma_+(t) = (\cos\alpha - 1)\,\frac{\omega t}{2}$$

or, for a complete cycle $T = \frac{2\pi}{\omega}$,

$$\gamma_+(T) = \pi(\cos\alpha - 1)$$

In a more general case, in which the tip of the $\vec{B}(t)$ vector sweeps out an arbitrary shape we get $\gamma_+(T) = -\frac{1}{2}\Omega$ where Ω is the solid angle subtended at the origin

Let us show it ...

The eigenstate with spin up along $B(t)$ is

$$\chi_+ = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix}$$

The gradient of χ_+ in spherical coordinates

$$\nabla\chi_+ = \left(\frac{\partial}{\partial r}\vec{e}_r + \frac{1}{r}\frac{\partial}{\partial\theta}\vec{e}_\theta + \frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}\vec{e}_\phi\right)\chi_+ =$$

$$= \frac{1}{r}\begin{pmatrix} -\frac{1}{2}\sin\frac{\theta}{2} \\ \frac{1}{2}e^{i\phi}\cos\frac{\theta}{2} \end{pmatrix}\vec{e}_\theta + \frac{1}{r\sin\theta}\begin{pmatrix} 0 \\ ie^{i\phi}\sin\frac{\theta}{2} \end{pmatrix}\vec{e}_\phi$$

Then

$$\langle\chi_+|\nabla\chi_+\rangle = \cancel{-\frac{1}{2r}\cos\frac{\theta}{2}\sin\frac{\theta}{2}\vec{e}_\theta + \frac{1}{2r}\sin\frac{\theta}{2}\cos\frac{\theta}{2}\vec{e}_\theta} + \frac{i}{r\sin\theta}\sin^2\frac{\theta}{2}\vec{e}_\phi$$

The curl in spherical coordinates is

$$\operatorname{curl}\vec{A} = \frac{1}{r\sin\theta}\left(\frac{\partial}{\partial\theta}(A_\phi\sin\theta) - \frac{\partial A_\theta}{\partial\phi}\right)\vec{e}_r + \frac{1}{r}\left(\frac{1}{\sin\theta}\frac{\partial A_r}{\partial\phi} - \frac{\partial}{\partial r}(rA_\phi)\right)\vec{e}_\theta + \frac{1}{r}\left(\frac{\partial}{\partial r}(rA_\theta) - \frac{\partial A_r}{\partial\theta}\right)\vec{e}_\phi \qquad \vec{A} = \begin{pmatrix} A_r \\ A_\theta \\ A_\phi \end{pmatrix}$$

In our case only the ϕ-component is nonzero, so

$$\nabla\times\langle\chi_+|\nabla\chi_+\rangle = \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}\left(\frac{i\sin^2\frac{\theta}{2}}{\sin\theta}\sin\theta\right)\vec{e}_r = \frac{i}{2r^2}\vec{e}_r$$

Then

$$\gamma_+(T) = i\int[\nabla\times\langle\chi_+|\nabla\chi_+\rangle)\cdot d\vec{S}$$

The integral is over the are of a sphere swept out by $\vec{B}(t)$ over one cycle, so $d\vec{S} = r^2 d\Omega\,\vec{e}_r$. Then

$$\gamma_+(T) = -\frac{1}{2}\int\frac{1}{r^2}\vec{e}_r\cdot r^2 d\Omega\,\vec{e}_r = -\frac{1}{2}\int d\Omega = -\frac{1}{2}\Omega$$